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A method for construction of symmetry diagram of space group

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Abstract : The symmetry operations of the space group as shown in its Hermann-Mauguin symbol are represented by 4×4 matrix. The unknowns are inserted at those positions in the fourth column which define the origin. The matrices are multiplied among themselves to generate new symmetry operations if any The unknowns are determined by origin fixing rules as described in International Tables for Crystallography, Volume 1. Each symmetry operation is combined with the lattice translation of the space group. This produces symmetry operations either of the same type or different type The symmetry elements are placed at their appropriate positions and the diagram is completed. The method is illustrated by many examples

Keywords : Space groups, crystal symmetry, theoretical crystallography

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1. Introduction

The 230 space groups in three dimensions were derived independently by Federov [1] in Russia and Schonflies [2] in Germany. They were studied in great details by Niggli [3] and Wyckoff [4] and later were published as Tables entitled Internationale Taballen zur Bestimmung von Kristallstrukturan under the editorship of Hermann [5]. The tables were prepared in great details as the knowledge of symmetry grew as International Tables for Crystallography (IT hereafter) [6,7].

Space groups have been presented by many authors using different methods at different level of complexity [8–15]. Computers have played a major role in the generation and preparation of space group information [16–18]. Hermann [19] and Mauguin [20] have devised convenient notations for space groups, known as Hermann-Mauguin symbols (H-M or International symbols) which are widely used by the crystallographic community all over the world. The notation contains an alphanumeric character which specifies the Bravais lattice type, the essential symmetry elements and their orientation with respect to the unit cell axes. The specification of origin is an essential information, needed to understand the space group diagram. Space groups are useful in structural crystallography and many branches of Physics. Wondratschek and Neubüser [21] have given a method to identify the symmetry operation from the equivalent positions as listed in IT [6].

In this paper, a method is presented to draw the symmetry diagram of a space group from its Hermann-Mauguin symbol. As a first step, the symmetry operations as shown in the symbol are represented by 4 × 4 matrix and then the method is described in a sequence of certain steps to be followed. A sufficient number of examples are described to illustrate the method.

2. Mathematical preliminaries

Space group symmetry operations are isometric mappings in E^3 which map a crystal pattern onto itself. The mappings maintain parallelism of straight lines and preserve distances. Referred to a coordinate system, the mappings or transformations may be written as

$$\begin{aligned} x_1' &= A_{11}x_1 + A_{12}x_2 + A_{13}x_3 + a_1, \\ x_2' &= A_{21}x_1 + A_{22}x_2 + A_{23}x_3 + a_2, \\ x_3' &= A_{31}x_1 + A_{32}x_2 + A_{33}x_3 + a_3. \end{aligned} \tag{1}$$

In abbreviated form, eqs. (1) may be expressed as

$$\boldsymbol{x}' = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{a} = (\boldsymbol{A},\boldsymbol{a})\boldsymbol{x} = (\boldsymbol{A}|\boldsymbol{a})\boldsymbol{x}, \tag{2}$$

where $\boldsymbol{x}'$, $\boldsymbol{x}$ and $\boldsymbol{a}$ are all (3 × 1) column matrices and $\boldsymbol{A}$ is an (3 × 3) square matrix and $\boldsymbol{x}' = (x_1', x_2', x_3')$ is the image of $\boldsymbol{x}$ $(= x_1, x_2, x_3)$ and $(A|a)$ is called the Seitz symbol. The mapping is invertible, *i.e.* for a given motion $M : x \rightarrow x'$, the inverse motion $M^{-1} : x' \rightarrow x$, exists and it is unique.

If $M = (A, a)$, then $M^{-1} = (A,a)^{-1} = (A^{-1}, -A^{-1}a)$.

The system of equations $x' = Ax + a$ may be conveniently represented into 4 × 4 matrix form for computational purpose or for extension to higher dimensions as

$$\begin{bmatrix} x_1' \\ x_2' \\ x_3' \\ \hline 1 \end{bmatrix} = \left[\begin{array}{ccc|c} A_{11} & A_{12} & A_{13} & a_1 \\ A_{21} & A_{22} & A_{23} & a_2 \\ A_{31} & A_{32} & A_{33} & a_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right] \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \hline 1 \end{bmatrix}. \tag{3}$$

The symmetry operation in (3) may be expressed in the form

$$(A,a) = \left[\begin{array}{ccc|c} a_{11} & a_{12} & a_{13} & a_1 \\ a_{21} & a_{22} & a_{23} & a_2 \\ a_{31} & a_{32} & a_{33} & a_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right]. \tag{4}$$

The matrix A depends on symmetry and the choice of basis vectors and the column a depends both on choice of basis vectors and the origin. The elements of A can take values 0 and ± 1 in suitable coordinate system whereas a_i are fraction of crystal unit cell length as 0, 1/6, 1/4, 1/3, 2/3, 1/2, 3/4 or 5/6. The successive application of the operation in (1) is described by the product of the corresponding 4×4 matrices. The set of all symmetry operations of an infinite crystal pattern forms the space group G of the crystal pattern. Owing to the periodicity in a crystal pattern, the translations are included among its symmetry operations. The infinitely many translation vectors of a space group in any dimension, form its space lattice. The space groups are infinite groups.

A point is called a fixed point of the mapping M if it is invariant under the mapping *i.e.*, $x'_f = x_f$. It may alternatively be called as a point on the symmetry element. It may be determined by solving the equation

$$(A,a)x_f = x_f, \tag{5}$$

The solution consists of a plane of points for a reflection, a line of points for rotation and a point for inversion or roto-inversion. No solution exists for translations. screw rotations and glide reflections. In such cases points on the symmetry elements may be obtained by solving the equation

$$(A, a - \hat{a})x_f = x_f, \tag{6}$$

where $\hat{a} = (A^{m-1} + A^{m-2} + \ldots\ldots + A + I)/m$ is the intrinsic part of the translation motion of the screw or glide symmetry operation, $A^m = I$, m being an integer and I is the unit matrix. The operation $(A, a - \hat{a})$ is a rotation or reflection only, the fixed point of which are used to characterize the original screw rotation or glide reflection.

In the following, a useful theorem is proved which generates more symmetry elements as a result of combination of rotation (screw rotation), reflection (glide-reflection) with the lattice translation.

Theorem 1 : A rotation about an axis through an angle α, followed by a translation t perpendicular to the axis, is equivalent to a rotation through the same angle α in the same sense, but about an axis B on the bisector AA' at a distance $t/2 \cot \alpha/2$ from AA', where A' is the translation equivalent lattice point.

Proof : Let α be a rotation about an axis A, followed by a translation t perpendicular to A (Figure 1).

Consider a point M_1. The rotation A_α brings M_1 to M_2, which is symmetrically situated on either side of perpendicular through A. The translation t brings M_2 to M_3. The intersection of AM_1 and $A'M_3$, the point B is unmoved. The net motion is therefore. equivalent to a rotation α (counterclockwise) about B (Figure 1). This may be stated as

$$A_\alpha \cdot T_\perp = \left[\begin{array}{ccc|c} \cos\alpha & -\sin\alpha & 0 & 0 \\ \sin\alpha & \cos\alpha & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right] \left[\begin{array}{ccc|c} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right] = \left[\begin{array}{ccc|c} \cos\alpha & -\sin\alpha & 0 & 1 \\ \sin\alpha & \cos\alpha & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right] = B_r \tag{7}$$

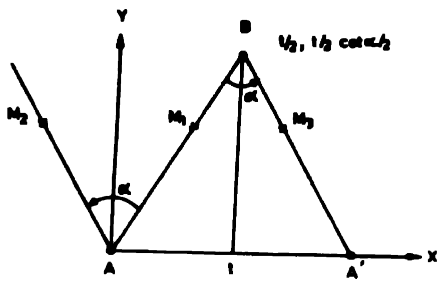

Figure 1. Combination of rotation A_α with a perpendicular translation $T_\perp$

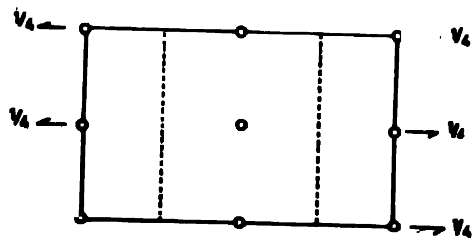

Figure 2. Space group diagram $P12_1/c\,1$ as projected down [001] direction

The coordinates of B on the symmetry axis may be determined by solving the equations

$$\left[\begin{array}{ccc|c} \cos\alpha & -\sin\alpha & 0 & t \\ \sin\alpha & \cos\alpha & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right] \left[\begin{array}{c} x_{1f} \\ x_{2f} \\ x_{3f} \\ \hline 1 \end{array}\right] = \left[\begin{array}{c} x_{1f} \\ x_{2f} \\ x_{3f} \\ \hline 1 \end{array}\right] \tag{8}$$

Expanding (8), we get

$$x_{1f}\cos\alpha - x_{2f}\sin\alpha + t = x_{1f}, \tag{9}$$

$$x_{1f}\sin\alpha + x_{2f}\cos\alpha = x_{2f}, \tag{10}$$

$$x_{3f} = x_{3f}. \tag{11}$$

Eqs. (9) to (11) admit a solution as

$$x_{1f} = t/2, \tag{12}$$

$$x_{2f} = t/2\cot\alpha/2, \tag{13}$$

$$x_{3f} = x_{3f}. \tag{14}$$

This proves the theorem.

Cor. 1. A combination of a rotation and a general translation gives rise to a screw motion, for

$$A_\alpha . T = A_\alpha . T_\perp . T_\parallel = B_\alpha . T_\parallel = B_{\alpha,T} \tag{15}$$

Cor. 2. A combination of a screw motion and a general translation gives rise to a screw motion with enhanced pitch, for

$$A_{\alpha,\tau} . T = A_{\alpha,\tau} . T_\perp . T_\parallel = B_{\alpha,\tau} . T_\parallel = B_{\alpha,\tau+T}. \tag{16}$$

The theorem also holds when A is an inversion or roto-inversion.

3. Choice of origin

The following rules are followed for fixing the origin (See p. 21 [6]).

i. All centrosymmetric space groups are described with inversion center at the origin. Sometime a point of higher site symmetry is chosen as the origin which does not coincide with the center of symmetry.

ii. For non-centrosymmetric space groups, the origin is chosen at a point of highest site symmetry. If no site symmetry is higher than one, the origin is placed on a screw axis or on a glide plane, or at the intersection of several such symmetry elements. Exceptions occur in several space groups.

4. Construction of symmetry diagram of space group

The following procedure is adopted for constructing the space group diagram :

1. Consider the Hermann-Mauguin symbol of the space group. Express the symmetry operations of the space group into 4×4 matrix form. The additional symmetry elements are a product of symmetry operations with lattice translations. The symmetry operations A and TA may be of the same nature and only the locations of their symmetry elements differ. The symmetry operations A and TA are of different nature and have different symbols corresponding to rotation or screw axes, to mirror or glide planes of different nature respectively.
2. Add unknowns in the last column of the matrix which are origin-dependent. The unknowns are determined by fixing the origin with the rules for the choice of origin.
3. Apply Theorem 1 or its corollary to combine symmetry operations with lattice translation to generate new symmetry elements within the unit cell.
4. Determine the fixed point for each symmetry element with the help of eqs. (5) or (6).
5. The symmetry diagram of the space group is drawn by placing the symmetry elements at their appropriate positions.

Examples :

(1) $P12_1/c1$

The space group is derived from point group $2/m$ in the monoclinic system and must be centrosymmetric. Accepting the convention that unique axis is the b-axis, the H-M symbol suggests the following symmetry operations :

Identity

$$(I|0,0,0) = \left[\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right] \tag{17}$$

2-fold screw axis

$$\left(2_1^+ \middle| \alpha, \frac{1}{2}, \beta\right) = \left[\begin{array}{ccc|c} \bar{1} & 0 & 0 & \alpha \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & \bar{1} & \beta \\ \hline 0 & 0 & 0 & 1 \end{array}\right]. \tag{18}$$

c-glide

$$\left(c \middle| 0, \gamma, 1/2\right) = \left[\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & \gamma \\ 0 & 0 & 1 & 1/2 \\ \hline 0 & 0 & 0 & 1 \end{array}\right]. \tag{19}$$

Multiplying (18) with (19) we get,

$$\left(\bar{1} \middle| \alpha, \tfrac{1}{2}+\gamma, -\tfrac{1}{2}+\beta\right) = \left[\begin{array}{ccc|c} \bar{1} & 0 & 0 & \alpha \\ 0 & \bar{1} & 0 & \frac{1}{2}+\gamma \\ 0 & 0 & \bar{1} & -\frac{1}{2}+\beta \\ \hline 0 & 0 & 0 & 1 \end{array}\right]. \tag{20}$$

It is an inversion center and by the rule (1), origin lies over it. This gives $\alpha = 0$, $\beta = \frac{1}{2}$, $\gamma = -\frac{1}{2}$ or $+\frac{1}{2}$.

Determination of the points on the symmetry elements

2_1 screw axis :

$$\left[\begin{array}{ccc|c} \bar{1} & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & \bar{1} & 1/2 \\ \hline 0 & 0 & 0 & 1 \end{array}\right] \left[\begin{array}{c} x_f \\ y_f \\ z_f \\ \hline 1 \end{array}\right] = \left[\begin{array}{c} x_f \\ y_f \\ z_f \\ \hline 1 \end{array}\right]. \tag{21}$$

Solving (21) we get $x_f = 0$ and $z_f = \frac{1}{4}$. The location of 2_1-axis is $0, y, \frac{1}{4}$ and is parallel to y-axis. The combination of 2_1 and perpendicular translation gives an equivalent 2_1-axis at $\frac{1}{2}, y, \frac{1}{4}$.

c-glide :

Point on the symmetry element is obtained by solving the equation

$$\left[\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \\ \hline 0 & 0 & 0 & 1 \end{array}\right] \left[\begin{array}{c} x_f \\ y_f \\ z_f \\ \hline 1 \end{array}\right] = \left[\begin{array}{c} x_f \\ y_f \\ z_f \\ \hline 1 \end{array}\right]. \tag{22}$$

This gives $x_f = x_f$, $y_f = \frac{1}{4}$ and $z_f = z_f + \frac{1}{2}$. It is located at $(x, \frac{1}{4}, z)$. Lattice translation perpendicular to glide will generate another glide at $(x, \frac{3}{4}, z)$. The combination of inversion center at (0, 0, 0) with lattice translations will generate inversions at $(\frac{1}{2}, 0, 0)$, $(0, \frac{1}{2}, 0)$, $(0, 0, \frac{1}{2})$, $(\frac{1}{2}, \frac{1}{2}, 0)$, $(0, \frac{1}{2}, \frac{1}{2})$, $(\frac{1}{2}, 0, \frac{1}{2})$ and $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. The symmetry diagram as projected down [001] is shown in Figure 2.

(2) *Pbca*

The space group is derived from point group *mmm*. It is a centrosymmetric space group in the orthorhombic system. The following symmetry operations are suggestive from its Hermann-Mauguin symbol :

$$\left(1 \middle| 0, 0, 0\right) = \left[\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right]; \qquad \left(b \middle| \alpha, \tfrac{1}{2}, 0\right) = \left[\begin{array}{ccc|c} \bar{1} & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 1 & 1 \end{array}\right]; \tag{23}$$

$$\left(c \middle| 0, \beta, \tfrac{1}{2}\right) = \left[\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & \beta \\ 0 & 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right]; \qquad \left(a \middle| \tfrac{1}{2}, 0, \gamma\right) = \left[\begin{array}{ccc|c} 1 & 0 & 0 & \frac{1}{2} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \bar{1} & \gamma \\ \hline 0 & 0 & 0 & 1 \end{array}\right]. \tag{23a}$$

Multiplying the last three matrices, we get

$$\left(\bar{1} \middle| 0, 0, 0\right) = \left[\begin{array}{ccc|c} \bar{1} & 0 & 0 & -\frac{1}{2}+\alpha \\ 0 & \bar{1} & 0 & \frac{1}{2}+\beta \\ 0 & 0 & \bar{1} & \frac{1}{2}+\gamma \\ \hline 0 & 0 & 0 & 1 \end{array}\right]. \tag{24}$$

Since the origin is chosen at the center of inversion, $\alpha = 1/2$, $\beta = 1/2$ or $-1/2$ and $\gamma = 1/2$ or $-1/2$. Determination of points on the symmetry elements indicate that *b* glide is located at

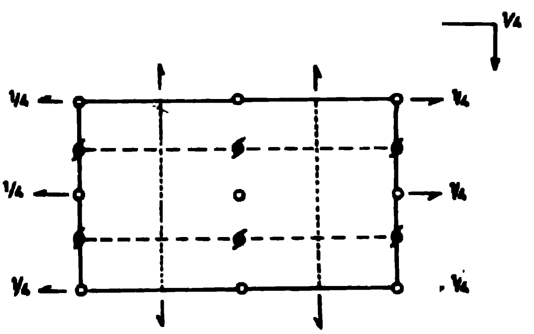

Figure 3. Space group diagram *Pbca* as projected down [001] direction.

(1/4, *y*, *z*), *c* glide at (*x*, 1/4, *z*) and *a* glide at (*x*, *y*, 1/4) The additional glides are produced at (3/4, *y*, *z*), (*x*, 3/4, *z*) and (*x*, *y*, 3/4) as a result of combination of lattice translations. The combination of two glides taken at a time produces 2_1 at (1/4, 0, *z*), (*x*, 1/4, 0) and

-(0, y, 1/4). In a similar way, center of inversions are generated half the cell edge, intersection of face diagonals and body diagonals. Figure 3 shows the projection of symmetry diagram along [001] direction.

(3) $P31c$

The space group is derived from the point group $3m$. It is a noncentrosymmetric space group in the rhombohedral system. According to the rule (ii) origin is chosen on $31c$. The following symmetry operations are suggestive of its Hermann-Mauguin symbol :

$$(1|0,0,0)=\left[\begin{array}{ccc|c}1&0&0&0\\0&1&0&0\\0&0&1&0\\\hline 0&0&0&1\end{array}\right] \text{ at } 0,0,z; \quad (3^+|0,0,0)=\left[\begin{array}{ccc|c}0&\bar{1}&0&0\\1&\bar{1}&0&0\\0&0&1&0\\\hline 0&0&0&1\end{array}\right] \text{ at } 0,0,z; \quad (25)$$

$$(3^-|0,0,0)=\left[\begin{array}{ccc|c}\bar{1}&1&0&0\\\bar{1}&0&0&0\\0&0&1&0\\\hline 0&0&0&1\end{array}\right] \text{ at } 0,0,z;$$

$$\begin{aligned} t(1,0,0).(3^+|0,0,0) &= (3^+|0,0,0) \text{ at } 2/3,1/3,z, \\ t(1,0,0).(3^-|0,0,0) &= (3^-|0,0,0) \text{ at } 2/3,1/3,z; \\ t(1,1,0).(3^+|0,0,0) &= (3^+|0,0,0) \text{ at } 1/3,2/3,z, \\ t(1,1,0).(3^-|0,0,0) &= (3^-|0,0,0) \text{ at } 1/3,2/3,z \end{aligned} \quad (26)$$

The glide reflection at $x0z$ implies another glide reflection plane at xxz. The angle between the two glide planes is 60°. The matrices for these two glide planes are

$$c\left|0,0,\tfrac{1}{2}\right) = \left[\begin{array}{ccc|c}1&\bar{1}&0&0\\0&\bar{1}&0&0\\0&0&1&\frac{1}{2}\\\hline 0&0&0&1\end{array}\right] \text{ at } x,0,z; \quad \left(c\left|0,0,\tfrac{1}{2}\right.\right) = \left[\begin{array}{ccc|c}0&1&0&0\\1&0&0&0\\0&0&1&\frac{1}{2}\\\hline 0&0&0&1\end{array}\right] \text{ at } x,x,z. \quad (27)$$

The combination (3 | 0, 0, 0). (c| 0, 0, $\frac{1}{2}$) at x, 0, z is equivalent to (c| 0, 0, $\frac{1}{2}$) at 0, y, z. The additional symmetry operations are obtained by combining the glide symmetry operations in (27) with lattice translations t (1, 0, 0) and t (0, 1, 0) respectively as

$$t(1,0,0).\{c|0,0,\frac{1}{2};y,0,z\} = \{n|-\frac{1}{2},0,\frac{1}{2};x,\frac{1}{2},z\}, \quad (28)$$

$$t(0,1,0).\{c|0,0,\frac{1}{2};x,0,z\} = \{n|0,\frac{1}{2},\frac{1}{2};\frac{1}{2},y,z\}. \quad (29)$$

The c glide located at x, x, z implies an n glide in x, $1/2 + x$, z with glide components $\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$ [22]. Figure 4 shows the projection of symmetry diagram along [001] direction.

(4) *P422*

The point group of the space group is 422. As the space group is noncentrosymmetric, the origin is chosen at the point of highest site symmetry 422.

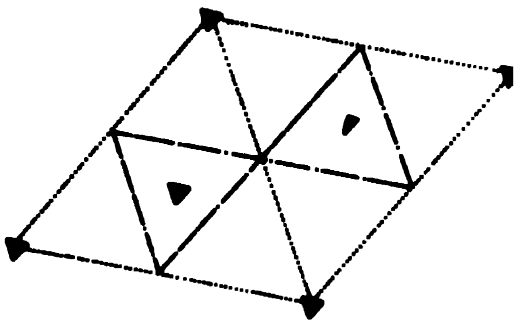

Figure 4. Space group diagram *P*13c as projected down [001] direction

The 4-fold axis is along [001] direction. The 2-fold axes are along [100] and [110] directions. The symmetry operations are

$$0,0,0) = \left[\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right] \qquad \left(4^{+} \mid 0,0,0\right) = \left[\begin{array}{ccc|c} 0 & \bar{1} & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right] \text{ at } (0,0,z);$$

$$\left(4^{-} \mid 0,0,0\right) = \left[\begin{array}{ccc|c} 0 & 1 & 0 & 0 \\ \bar{1} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right] \text{ at } (0,0,z); \quad \left(2 \mid 0,0,0\right) = \left[\begin{array}{ccc|c} \bar{1} & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right] \text{ at } (0,0,z)$$

$$\left(2 \mid 0,0,0\right) = \left[\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right] \text{ at } (x,0,0); \quad \left(2 \mid 0,0,0\right) = \left[\begin{array}{ccc|c} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & \bar{1} & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right] \text{ at } (x,x,0). \tag{30}$$

The combination of above symmetry operations with lattice translations t (1,0,0), t (1,1,0) and t (0,1,0) gives additional symmetry operations :

$$\begin{aligned}
t(1,0,0)\cdot\left\{(4 \mid 0,0,0);\ 0,0,z\right\} &= \left\{(4 \mid 0,0,0);\ \tfrac{1}{2},\tfrac{1}{2},z\right\}, \\
t(1,1,0)\cdot\left\{\left(4^{-1} \mid 0,0,0\right);\ 0,0,z\right\} &= \left\{\left(4^{-1} \mid 0,0,0\right);\ \tfrac{1}{2},\tfrac{1}{2},z\right\}, \\
t(1,0,0)\cdot\left\{(2 \mid 0,0,0);\ 0,0,z\right\} &= \left\{(2 \mid 0,0,0);\ \tfrac{1}{2},0,z\right\}, \\
t(0,1,0)\cdot\left\{(2 \mid 0,0,0);\ 0,0,z\right\} &= \left\{(2 \mid 0,0,0);\ 0,\tfrac{1}{2},z\right\}, \\
t(1,1,0)\cdot\left\{(2 \mid 0,0,0);\ 0,0,z\right\} &= \left\{(2 \mid 0,0,0);\ \tfrac{1}{2},\tfrac{1}{2},z\right\}, \\
t(1,0,0)\cdot\left\{(2 \mid 0,0,0);\ x,x,0\right\} &= \left\{\left(2_{1} \mid \tfrac{1}{2},\tfrac{1}{2},0\right);\ x,x+\tfrac{1}{2},0\right\}.
\end{aligned} \tag{31}$$

Figure 5 shows the projection of the diagram along [00ī] direction.

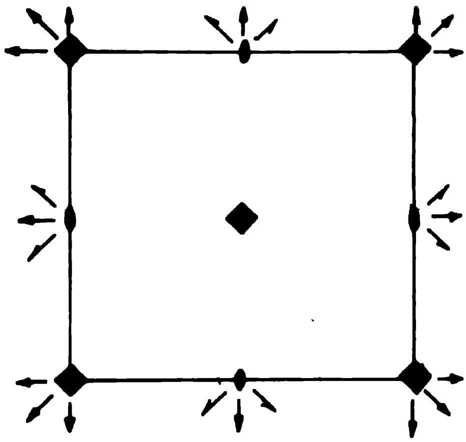

Figure 5. Space group diagram $P422$ as projected down [001] direction.

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